06/09/2007,10551574IIe.trn

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

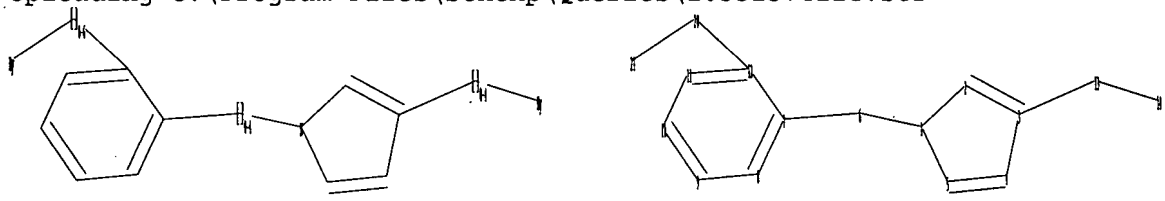
LOGINID:SSPTASXY1626

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 12:27:15 ON 06 SEP 2007
FILE 'REGISTRY' ENTERED AT 12:27:15 ON 06 SEP 2007
COPYRIGHT (C) 2007 American Chemical Society (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	345.55	1547.24

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-22.62

=>
Uploading C:\Program Files\Stnexp\Queries\10551574IIe.str



chain nodes :
6 13 14 20 21
ring nodes :
1 2 3 4 5 7 8 9 10 11 12
chain bonds :
1-6 3-13 6-7 12-20 13-14 20-21
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 1-5 1-6 13-14 20-21
exact bonds :
2-3 3-4 3-13 4-5 6-7 12-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 : 7 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:Atom 20:CLASS 21:Atom
Generic attributes :
14:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7

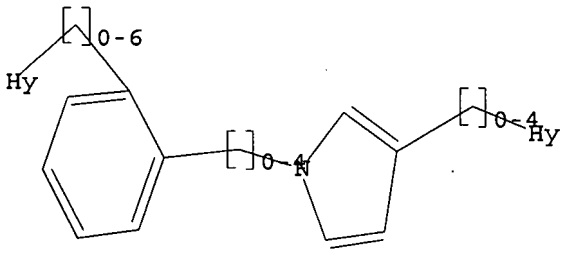
Number of Hetero Atoms : Exactly 1
Type of Ring System : Monocyclic

Element Count :
Node 14: Limited
N,N1
C,C5
O,O0
S,S0

Node 21: Limited
N,N1
C,C5
O,O0
S,S0

L37 STRUCTURE UPLOADED

=> d l37
L37 HAS NO ANSWERS
L37 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l37
SAMPLE SEARCH INITIATED 12:28:00 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 14385 TO ITERATE

13.9% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 280515 TO 294885
PROJECTED ANSWERS: 0 TO 0

L38 0 SEA SSS SAM L37

=> s l37 full
FULL SEARCH INITIATED 12:28:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 289422 TO ITERATE

100.0% PROCESSED 289422 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.03

L39 0 SEA SSS FUL L37

=> d l34
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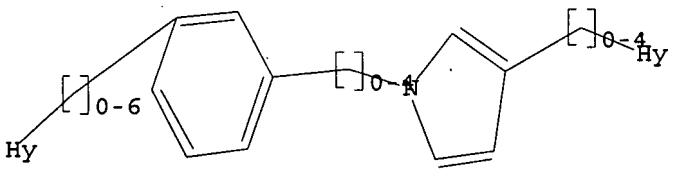
L34 STR



Structure attributes must be viewed using STN Express query preparation.

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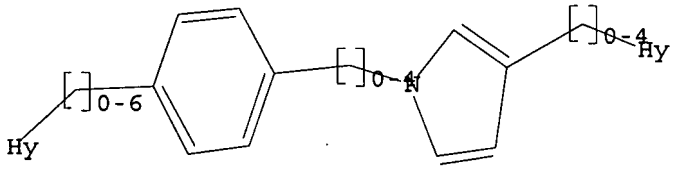
L31 HAS NO ANSWERS
L31 STR



Structure attributes must be viewed using STN Express query preparation.

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	518.55	1720.24

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-22.62

FILE 'HCAPLUS' ENTERED AT 12:28:48 ON 06 SEP 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

06/09/2007,10551574IIe.trn

FILE COVERS 1907 - 6 Sep 2007 VOL 147 ISS 11
FILE LAST UPDATED: 5 Sep 2007 (20070905/ED)

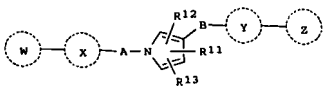
New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l33
L40   1 L33

=> d ed abs ibib hitstr tot

L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 21 Oct 2004
GI



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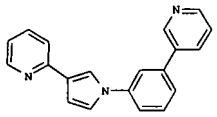


II

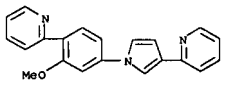
AB Title compds. represented by the formula I [wherein X, Y = independently (hetero)aryl, and at least one of X and Y is a heteroaryl with N adjacent to the position of attachment to A or B; A, B = independently (hetero)alkyl, alkylsulfonylalkyl, alkylcarbonylalkyl, etc.; W, Z = independently (un)substituted (hetero)cycloalkyl, alkyl(hetero)aryl; R11, R12, R13 = independently halo, alkyl, alkoxy, etc.; and pharmaceutically acceptable salts thereof] were prepared as modulators of metabotropic glutamate receptor-5 (mGluR5). For example, reaction of 2-(1H-pyrrol-3-yl)pyridine with 3-(3-iodophenyl)pyridine gave II. The prepared I were tested for mGluR5 inhibitory activity with IC50 value of less than 10 μM in the calcium flux assay or inhibition at a concentration of 100μM in the PI assay. Thus, I and their pharmaceutical compns. are useful as modulators of mGluR5 for the treatment of panic, and bipolar disorder, as well as in the treatment of psychiatric and mood disorders such as, for example, schizophrenia, anxiety, depression, panic, and bipolar disorder, as well as in the treatment of pain, Parkinson's disease, cognitive dysfunction, epilepsy, circadian rhythm disorders, obesity, drug addiction, drug abuse, drug withdrawal and other diseases (no data).

ACCESSION NUMBER: 2004:872663 HCAPLUS
DOCUMENT NUMBER: 141:366129
TITLE: Preparation of diaryl substituted pyrrole modulators of metabotropic glutamate receptor-5
INVENTOR(S): Cosford, Nicholas D. P.; Huang, Dehua; Roppe, Jeffrey R.; Smith, Nicholas D.; Tehrani, Lida R.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089308	A2	20041021	WO 2004-US9845	20040331
WO 2004089308	A3	20050922		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004227854	A1	20041021	AU 2004-227854	20040331
CA 2521399	A1	20041021	CA 2004-2521399	20040331
EP 1613265	A2	20060111	EP 2004-749565	20040331
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
CN 1794990	A	20060628	CN 2004-80014565	20040331
JP 2006522137	T	20060928	JP 2006-509518	20040331
US 2006193926	A1	20060831	US 2005-551574	20051003
PRIORITY APPLN. INFO.:			US 2003-460085P P	20030404
			WO 2004-US9845 W	20040331

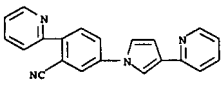
OTHER SOURCE(S): MARPAT 141:366129
IT 777863-51-1P 777863-57-7P 777863-66-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diaryl substituted pyrrole modulators of metabotropic glutamate receptor-5)
RN 777863-51-1 HCAPLUS
CN Pyridine, 2-[1-[3-methoxy-4-(2-pyridinyl)phenyl]-1H-pyrrol-3-yl]-, dihydrochloride (9CI) (CA INDEX NAME)



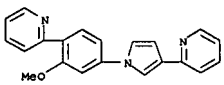
●2 HCl

RN 777863-57-7 HCAPLUS
CN Benzonitrile, 2-(2-pyridinyl)-5-[3-(2-pyridinyl)-1H-pyrrol-1-yl]- (9CI)

L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(CA INDEX NAME)



RN 777863-66-8 HCAPLUS
CN Pyridine, 2-[1-[3-methoxy-4-(2-pyridinyl)phenyl]-1H-pyrrol-3-yl]- (9CI) (CA INDEX NAME)



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=> s l36
L41             1 L36

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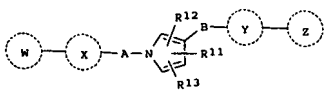
L41 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 21 Oct 2004
GI



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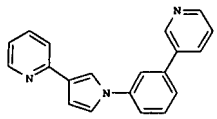

II

AB Title compds. represented by the formula I [wherein X, Y = independently (hetero)aryl, and at least one of X and Y is a heteroaryl with N adjacent to the position of attachment to A or B; A, B = independently (hetero)alkyl, alkylsulfonylalkyl, alkylcarbonylalkyl, etc.; W, Z = independently (un)substituted (hetero)cycloalkyl, alkyl(hetero)aryl; R11, R12, R13 = independently halo, alkyl, alkoxy, etc.; and pharmaceutically acceptable salts thereof] were prepared as modulators of metabotropic glutamate receptor-5 (mGluR5). For example, reaction of 2-(1H-pyrrol-3-yl)pyridine with 3-(3-iodophenyl)pyridine gave II. The prepared I were tested for mGluR5 inhibitory activity with IC50 value of less than 10 μM in the calcium flux assay or inhibition at a concentration of 100μM in the PI assay. Thus, I and their pharmaceutical compns. are useful as modulators of mGluR5 for the treatment of panic, and bipolar disorder, as well as in the treatment of psychiatric and mood disorders such as, for example, schizophrenia, anxiety, depression, panic, and bipolar disorder, as well as in the treatment of pain, Parkinson's disease, cognitive dysfunction, epilepsy, circadian rhythm disorders, obesity, drug addiction, drug abuse, drug withdrawal and other diseases (no data).

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DOCUMENT NUMBER: 141:366129
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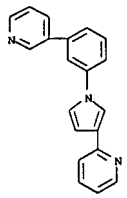
INVENTOR(S): Cosford, Nicholas D. P.; Huang, Dehua; Roppe, Jeffrey R.; Smith, Nicholas D.; Tehrani, Lida R.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

L41 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089308	A2	20041021	WO 2004-US9845	20040331
WO 2004089308	A3	20050922		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004227854	A1	20041021	AU 2004-227854	20040331
CA 2521399	A1	20041021	CA 2004-2521399	20040331
EP 1613265	A2	20060111	EP 2004-749565	20040331
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
CN 1794990	A	20060628	CN 2004-80014565	20040331
JP 2006522137	T	20060928	JP 2006-509518	20040331
US 2006193926	A1	20060831	US 2005-551574	20051003
PRIORITY APPLN. INFO.:			US 2003-460085P P	20030404
			WO 2004-US9845 W	20040331

OTHER SOURCE(S): MARPAT 141:366129
IT 777863-50-0P 777863-61-3P 777863-67-9P
777863-70-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diaryl substituted pyrrole modulators of metabotropic glutamate receptor-5)
RN 777863-50-0 HCAPLUS
CN Pyridine, 2-[1-[3-(3-pyridinyl)phenyl]-1H-pyrrol-3-yl]-, monohydrochloride
(9CI) (CA INDEX NAME)

L41 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

RN 777863-61-3 HCAPLUS
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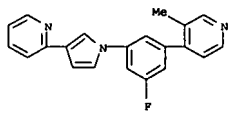
(9CI) (CA INDEX NAME)



RN 777863-67-9 HCAPLUS
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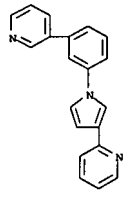

RN 777863-70-4 HCAPLUS
CN Pyridine, 3-[3-fluoro-5-[3-(2-pyridinyl)-1H-pyrrol-1-yl]phenyl]-4-methyl-

L41 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)